8th Int. Symp. "Nanostructures: Physics and Technology"
St Petersburg, Russia, June 19–23, 2000

Theoretical investigation of Auger recombination in spherical quantum dots

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Abstract. The principal mechanisms of Auger recombination (AR) of nonequilibrium carriers in spherical quantum dots (QDs) are investigated theoretically. It is shown that there exist two Auger recombination mechanisms of (i) quasithreshold and (ii) thresholdless types. These mechanisms originate from the existence of barriers but have different nature. The quasithreshold mechanism is caused by confinement of carriers within the region of a quantum dot which makes the quasimomentum conservation law approximate and enhances AR process. With increase of the dot radius this process turns to the threshold one. The thresholdless mechanism relates to the violation of the momentum conservation law at the heteroboundary and disappears with the radius tending to infinity.

1. Introduction

There are two main processes of Auger recombination (AR) in narrow gap semiconductors. The first of them corresponding to recombination of an electron and heavy hole and excitation another electron is the CHCC process. The second CHHS Auger process relates to the transition of a heavy hole to the spin-orbit split-off band. Contrary to bulk semiconductor in heterostructures the transversal momentum component doesn't conserve thus allowing the thresholdless Auger process to appear [1, 2]. In [3, 4] it was shown that there are three types of AR processes in quantum wells (QWs): (i) threshold, (ii) quasithreshold, (iii) thresholdless; and there are two types of AR processes in quantum wires (QWRs): (i) quasithreshold and (ii) thresholdless mechanisms [5, 6]. The AR mechanism of thresholdless type in a QWR differs from those in a QW because there are two different channels (i) with transfer of a large linear momentum to the excited electron (like in planar QWs) and (ii) with transfer of an angular momentum. The later channel was predicted to be the only possible channel for quantum dots [5, 6]. The forthcoming analysis shows that there are similar mechanisms of AR in spherical semiconductor QDs.

2. Theoretical model

The Auger recombination (AR) in bulk semiconductor was investigated several decades ago [7, 8]. It was shown that Auger process calculated in the first order of perturbation theory on Coulomb interaction has a threshold nature, i.e. its coefficient exponentially depends on temperature. For the calculation of the coefficients of the two main processes of AR: CHCC and CHHS it is necessary to work in framework of the multi-band $\underline{k}p$-theory, because complex valence band structure is necessary for the correct description of the CHHS process and the parabolicity of the spectrum in the conduction band is too rough approximations for the electron with the energy $E \approx E_g$.

We work in 8-band Kane's model with finite constant of spin-orbit interaction Δ_{so}. It is convenient to take basis wave function in the conduction and valence band in form of eigenfunction of the angular momentum [9]:

$$|0\uparrow\rangle, |0\downarrow\rangle, |1,1\uparrow\rangle, |1,1\downarrow\rangle, |1,0\uparrow\rangle, |1,0\downarrow\rangle, |1,-1\uparrow\rangle, |1,-1\downarrow\rangle \quad (1)$$

This procedure excretes eigenfunctions having definite angular momentum and corresponding to the spherical symmetry of the QD.

3. Eigenstates of carriers in a quantum dot

Commonly, the eigenstates of carriers in a QD is deriving from the elimination the wave functions at the interface which corresponds to the infinite heights of heterobarriers [9].

We derive boundary conditions from the continuity of the transversal component of the probability flux density. These boundary conditions correspond to the finite offsets in the conduction and valence bands V_c and V_v, respectively.

In limit $\Delta_{so} \to \infty$ these boundary correspond to common boundary conditions in 4-band Kane model, i. e.:

$$f_l^<(r=R) = f_l^>(r=R), \frac{1}{2E+E_g^d}\frac{df_l^<(r=R)}{dr} = \frac{1}{2E+E_g^m}\frac{df_l^>(r=R)}{dr}, \quad (2)$$

where $f_l^<(r)$ and $f_l^>(r)$ are solutions of the radial wave equation inside and outside the QD, respectively, and the spatial dependence of $E_g(\mathbf{r})$ is given by a step function $E_g(\mathbf{r}) = E_g^d + \Theta(r-R)(E_g^m - E_g^d)$ [10, 11].

4. Matrix element of Auger recombination

The probability of AR per unit time can be calculated in terms of the first-order perturbation theory in electron-electron interaction:

$$W_{i\to f} = \frac{2\pi}{\hbar}|M_{fi}|^2 \delta(\varepsilon_f - \varepsilon_i), \quad (3)$$

where

$$M_{fi} = \left\langle \Psi_f(\mathbf{r_1}, \mathbf{r_2}, \nu_1, \nu_2) \left| \frac{e^2}{\kappa_\infty |\mathbf{r_1} - \mathbf{r_2}|} \right| \Psi_i(\mathbf{r_1}, \mathbf{r_2}, \nu_1, \nu_2) \right\rangle \quad (4)$$

is the matrix element of electron-electron interaction, $\mathbf{r_1}$ and $\mathbf{r_2}$ are carrier co-ordinates, ν_1 and ν_2 are spin variables, e is an electron charge, and κ_∞ is the permittivity of the intrinsic semiconductor [3, 4].

For the spherical QD it is essential to decompose the Coulomb interaction into the spherical harmonics, using following equation:

$$\frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{\mathbf{r_2}}{(2l+1)\mathbf{r_1}^{l+1}} Y_{lm}(\theta_1, \alpha_1) Y_{lm}^*(\theta_2, \alpha_2). \quad (5)$$

It is easy matter to see that the matrix element of AR automatically yields conservation laws for the angular momentum and z-component of angular momentum (where z is axis

corresponding to the second quantum number in our basis 1). After integration along angular coordinates matrix element takes simplier form:

$$M_{fi} = \frac{4\pi^2}{(2l+1)\epsilon_\infty} \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \chi_l(r_1, r_2) f_{1,4}(r_1) f_{2,3}(r_2), \tag{6}$$

where $f_{i,j}$ multiplication of radial components of corresponding wave functions and:

$$\chi_l(r_1, r_2) = \frac{\min(r_1, r_2)^l}{\max(r_1, r_2)^{l+1}}. \tag{7}$$

5. Rate of Auger recombination

To calculate the rate of AR in the first order of perturbation theory, the probabilities of transition should be averaged over all initial states of carriers with appropriate weight-occupation numbers and summed over all final states:

$$G = \frac{2\pi}{\hbar} \sum_{n_1,m_1,n_2,m_2,n_3,m_3,\mathbf{k}_4} \langle M^2 \rangle f_1 f_2 (1 - f_3)(1 - f_4) \delta(E_3 + E_4 - E_1 - E_2) \tag{8}$$

here f_1, f_2 are the occupancies of the initial states and f_3, f_4 are those of the final states, $\langle M^2 \rangle$ is the sum of squared Auger matrix elements over spins of the initial and final states. In this equation is proposed that the final state of excited particle 4 lies in continuous spectrum. It is obviously true in our approximation V_c, $V_v \ll E_g$.

6. Summary

Our analysis has shown that for the Auger processes in semiconductor structures with QDs there exist two different AR mechanisms: thresholdless and quasithreshold, similarly to the case of planar quantum wells and cylindrical quantum wires.

Acknowledgements

The authors would like to acknowledge the Russian Foundation for Basic Research (Grants 98-07-90336, 99-02-16796) for support of this work.

References

[1] G. G. Zegrya and V. A. Kharchenko, *Sov. Phys. JETP* **74**, 173 (1992).

[2] M. I. Dyakonov and V. Yu. Kachorovskii, *Phys. Rev.* **B 49**, 17 130 (1994).

[3] G. G. Zegrya and A. S. Polkovnikov, *Zh. Exp. Teor. Fiz.* **113**, 1491 (1998) [JETP **86**, 815 (1998)].

[4] A. S. Polkovnikov and G. G. Zegrya, *Phys. Rev.* **B58**, 4039 (1998).

[5] E. B. Dogonkine, G. G. Zegrya and A. S. Polkovnikov, *Zh. Exp. Teor. Fiz.* **117**, (2000) (at press).

[6] E. B. Dogonkine, A. S. Polkovnikov and G. G. Zegrya, *7th Int. Symp. Nanostructures: Physics and Technology*, St. Petersburg, Russia, June 14-18, p 42–45, 1999.

[7] A. R. Beattie and P. T. Lansberg, *Proc. Roy. Soc.* **A 249**, 16 (1959).

[8] B. L. Gel'mont, *Sov. Phys. JETP* **48**, 268 (1978).

[9] P. C. Sercel and K. J. Vahala, *Phys. Rev.* **B42**, 3690 (199?).

[10] D. I. Chepic, Al. L. Efros, A. I. Ekimov, M. G. Ivanov, V. A. Kharchenko, I. A. Kudriavtsev and T. V. Yazeva, *J. Lumin.* **47**, 113–127 (1990).

[11] V. A. Kharchenko and M. Rosen, *J. Lumin.* **70**, 158–179 (1996).